

Electronic Supplementary data for
Pyrenyl Substituted 1,8-Naphthalimide as a New Material for Weak
Efficiency-roll-off Red OLED: A Theoretical and Experimental Study

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Additional data of XRD analysis**Table S1.** Data of crystal analysis of compound **ImPy** structure.

Empirical Formula	C ₃₆ H ₃₁ NO ₂ xTHF
Crystal Color, Habit	yellow platelet
Crystal Dimensions	0.540 x 0.390 x 0.120 mm
Crystal System/ Lattice Type	triclinic
Lattice Parameters	a = 9.290(13) Å α = 78.37(4) ^o b = 12.67(2) Å β = 79.43(5) ^o c = 13.43(2) Å γ = 89.40(6) ^o V = 1521(4) Å ³
Space Group	P-1 (#2)
Z value	2
d _{calc}	1.113 g/cm ³
R1 ^a	0.1802
wR2 ^b	0.5179

^a $R1 = \sum ||Fo| - |Fc|| / \sum |Fo|$

^b $wR2 = [\sum (w (Fo^2 - Fc^2)^2) / \sum w(Fo^2)^2]^{1/2}$

Additional data of thermal analysis of **ImPy**

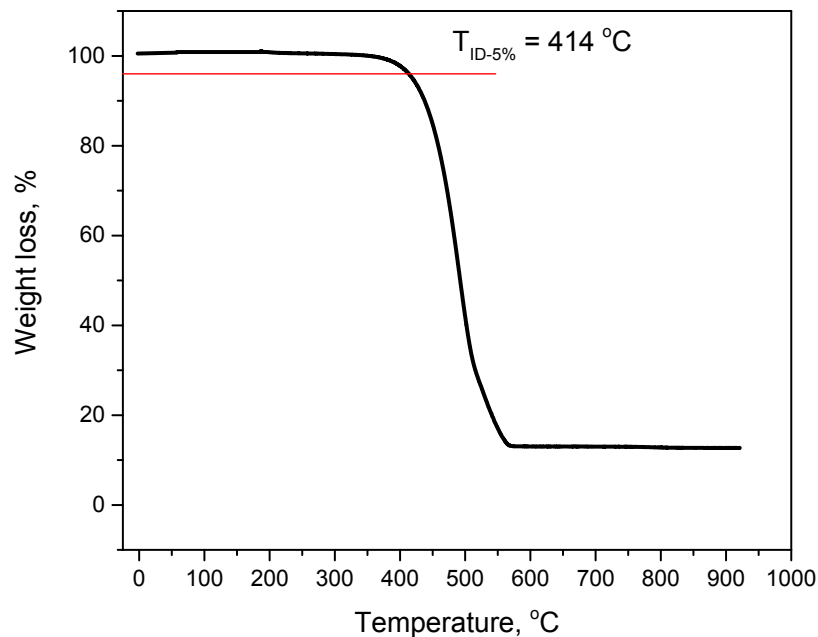


Fig. S1. TGA thermogram of compound **ImPy** (scan rate of 20 °C min^{-1} , N_2 atmosphere).

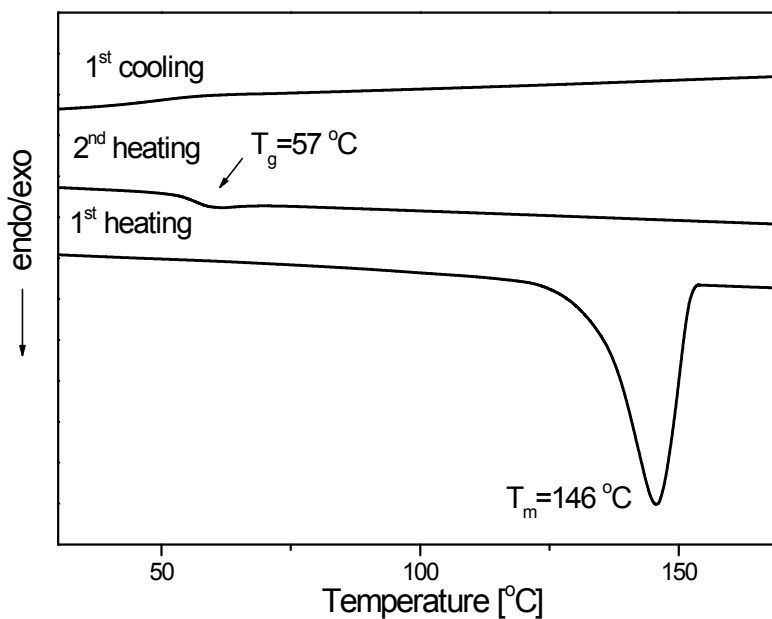


Fig. S2. DSC thermograms of compound **ImPy** (scan rate of 10 °C min^{-1} , N_2 atmosphere).

Additional data of electrical properties of ImPy

Table S2. Estimated distances between the acceptor and donor moieties, transfer integrals and external and internal reorganisation energies of the **ImPy** compound.

Entry	d_{D-D} / Å	d_{A-A} / Å	H(h ⁺) / H(e ⁻) / meV	$\lambda_{\text{ext}}(\text{h}^+)/$ meV	$\lambda_{\text{ext}}(\text{e}^-)/$ meV	-E _i / kJ mol ⁻¹
1	9.4	9.4	19/ 111	4.0/ 4.0		29.4
2	14.2	3.9	5.7/ 15.6	6.5/ 0		52.2
3	5.8	12.8	14.4/ 2.3	0/ 6.0		44.3
4	21.5	12.6	21/ 18	8.1/ 5.9		32.9

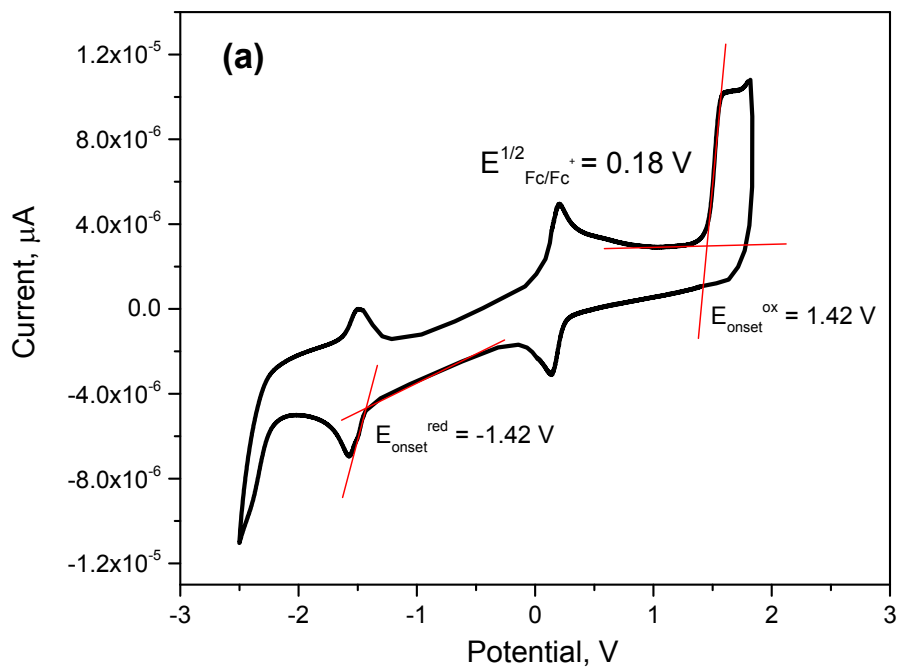


Fig. S3. Electrochemical cyclic voltammogram of **ImPy** in acetonitrile with 0.1 M TBAPF₆ supporting electrolyte at 50 mVs⁻¹ scan rate.

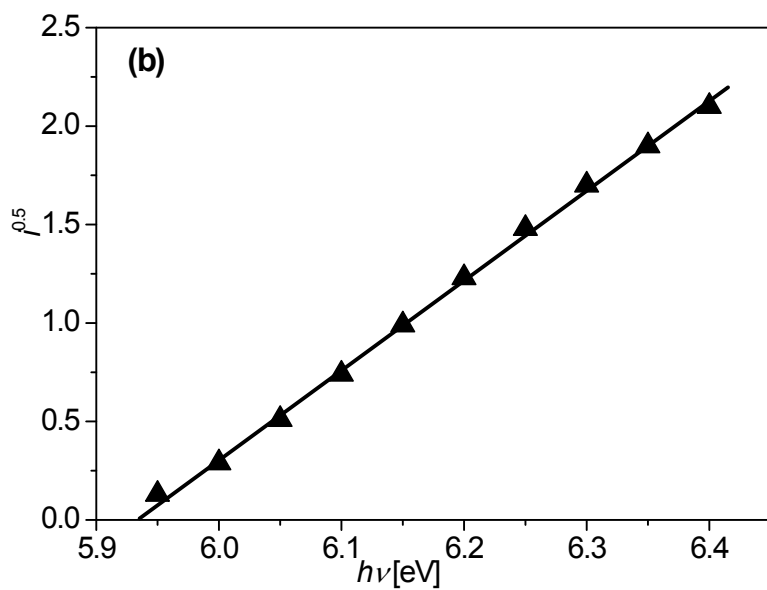


Fig. S4. Electron photoemission spectra of the layer of **ImPy**.

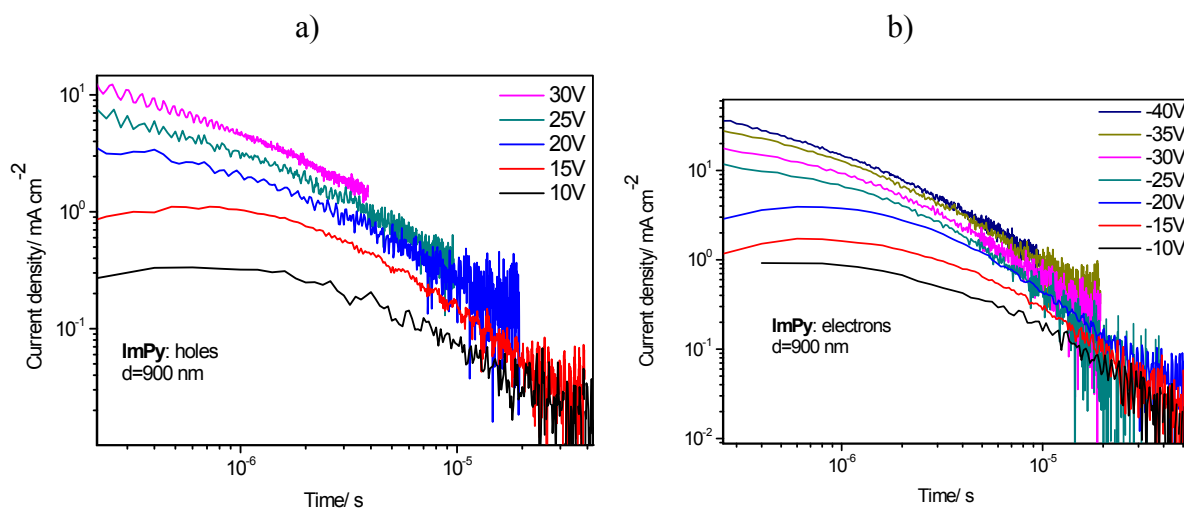


Fig. S5. TOF transients for hole (a) and electron (b) transport for compound **ImPy**.

Additional properties of electroemission

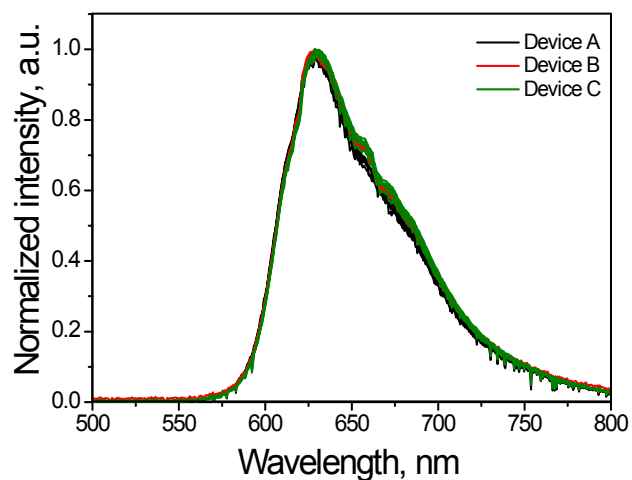


Fig. S6. Electroemission of A-C devices.

Table S3. Selected device performances.

Device	Structure	V_{on}^a / V	Max. brightness / Cd m^{-2}	Max. η_c / Cd A^{-1}	Max. η_p / Lm W^{-1}	Max. EQE/ %
A	ITO/MoO ₃ (/NPB /Ir(piq) ₂ (acac)(10%):ImPy /TPBi/LiF/Al	3.5	15300	10.8	7.1	13.6
B	ITO/MoO ₃ (/NPB /Ir(piq) ₂ (acac)(15%):ImPy /TPBi/LiF/Al	3.5	14900	9.7	6.6	12.6
C	ITO/MoO ₃ (/NPB /Ir(piq) ₂ (acac)(25%):ImPy /TPBi/LiF/Al	3.7	12000	5.2	2.7	7.0

a The operating voltage at a brightness of 1 Cd m^2 .

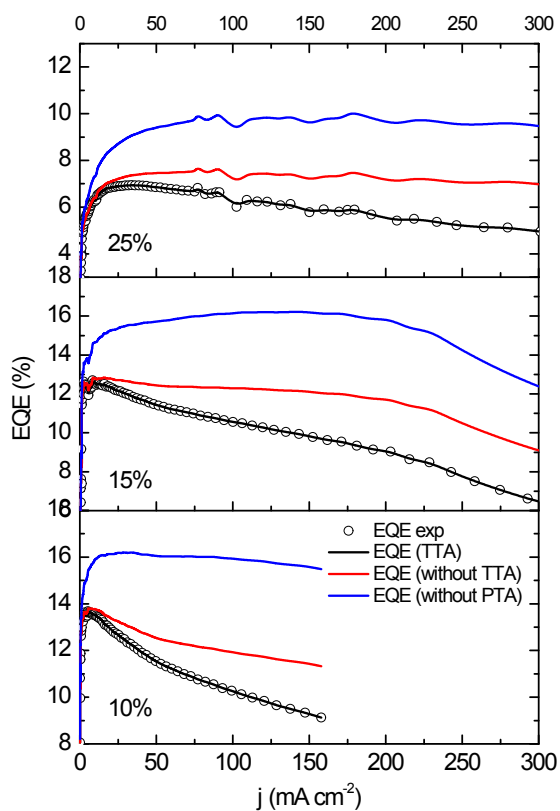
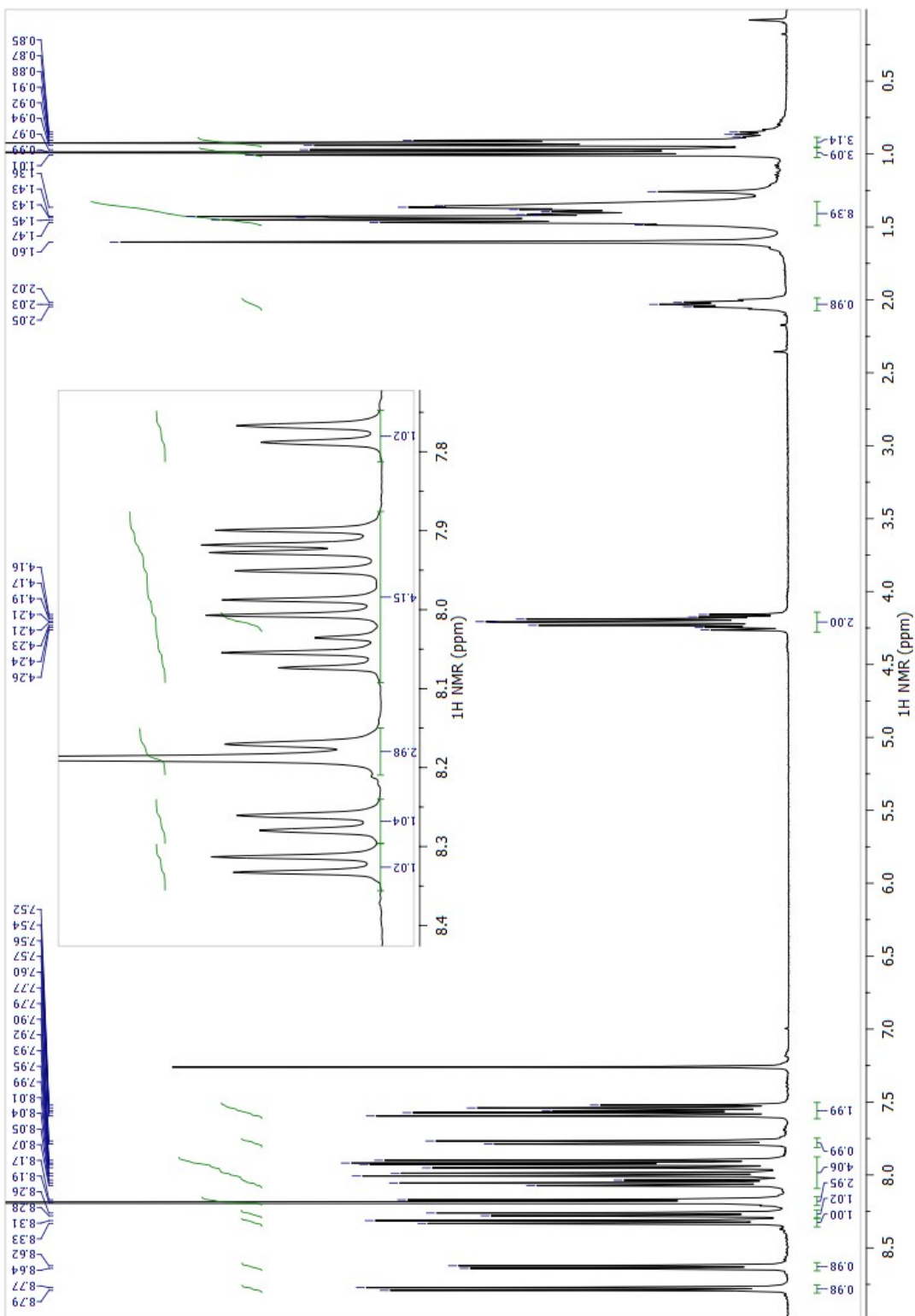


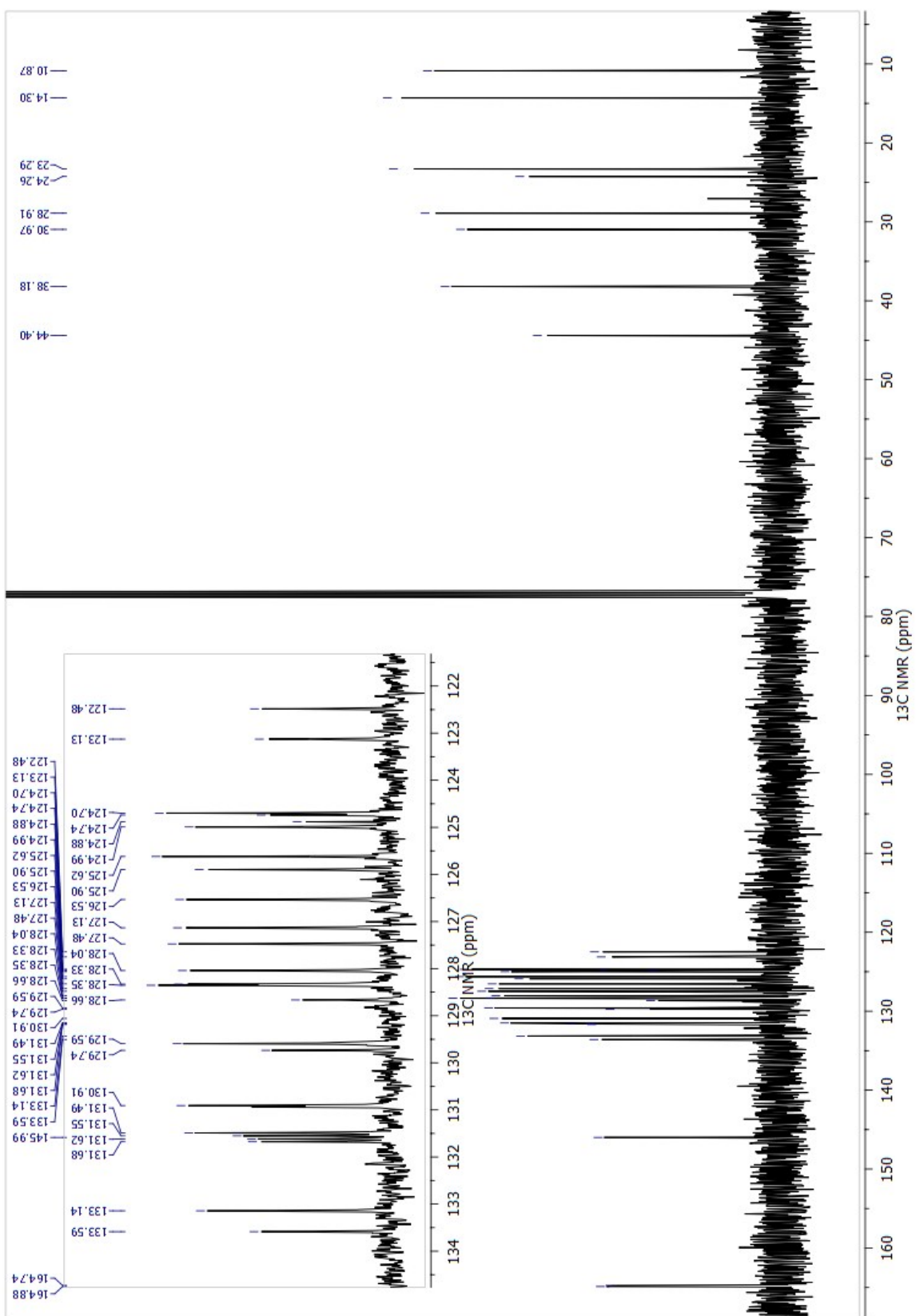
Fig. S7. Measured (scatter) and fitted EQE (black curves) versus the current density characteristics of the devices at the concentrations of 10, 15 and 25% of Ir(piq)₂(acac) in the host. The red curves represent EQE₀ in absence of TTA and the blue curves represent EQE₀ in absence of TPQ.

NMR, FT-IR and MS spectra of ImPy

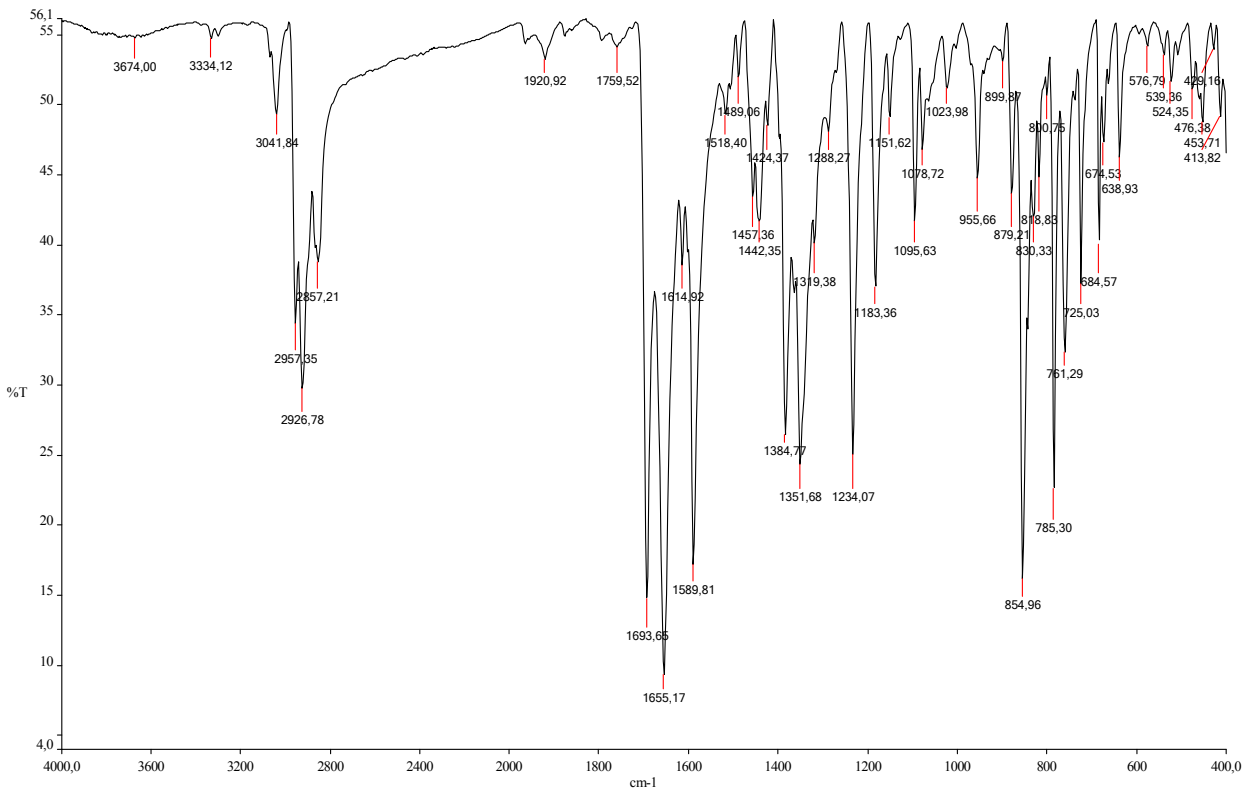
^1H -NMR of ImPy



¹³C-NMR of ImPy



FT-IR of ImPy



Mass of ImPy

